Multiplet Analysis Tool

This is a brief guide to multiplet analysis, a procedure to determine coupling between peaks, a useful tool in peak assignment. Note the MANAGUIDE command provides a basic flowchart, but it is often poorly worded, and the automation features can easily get confused.

1. Acquire a 1D NMR spectrum of the compound you wish to analyze. *nb:* All peaks and multiplets under consideration must be resolved.
2. Using the *Peak Pick* button, pick all the peaks to be analyzed. Any peaks not assigned in this way will be ignored. This is best done manually: the automatic peak-pick function is easily confused.
3. Enter Multiplet Analysis mode (MANA or *Analysis / Multiplet Analysis*).
4. Define the multiplets, from smallest to largest J, initially defining only the most basic splitting patterns (*eg*, only the triplets in a dt). This is best done manually, using the "define by region" button (3^{rd} from left), as the software is a poor judge of what constitutes a multiplet.
5. Couple existing multiplets by clicking the corresponding button (5^{th} button in). Select the multiplets to be coupled by clicking them (click again to deselect). Right click and select *define multiplet*; stop to marvel at your complex splitting pattern. Click the *couple existing multiplets* button twice if you wish to couple another set. Note that the software will only let you couple multiplets with the same splitting.
6. If you desire, right-click a multiplet and select *define identifiers* to give the multiplet a unique name.
7. Click the report button to list the multiplets and coupling constants.
8. Within the report, click *find connections*. You will be prompted to define threshold limits for difference in coupling constants. The standard values seem to work fine.
9. This report can be printed, copied, pasted, or saved to a text-file. It can also be loaded into the PLOT program, for inclusion on a spectrum.

Retyped from a report by Justin Spott '10.